A Multiscale 3D Simulation Of A Photocatalytic Reactor For Converting CO2 Into Hydrocarbons

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Abstract

In this paper, a multiscale 3D model is being built to simulate the heat and flow characteristics, as well as the macro- and micro- concentration distributions inside the HI-Light reactor - a solar-thermocatalytic "reverse combustion" technology that enables the conversion of CO2 and water to methanol and other high-value hydrocarbons, increasing its value as a commodity. The unique feature of our reactor is the simultaneous light and reactant delivery technique that maximizes utilization of catalyst in the reactor. This is accomplished through a novel variant on the traditional "shell-and-tube" reactor design where the tubes are internal light-guiding rods with specially designed scattering surfaces that enable deep and efficient penetration of the solar energy into the reactor, and the reagents and products flow through the shell outside the rods.

Different modules are being used in the present study: CFD Module and Heat Transfer Module to examine the heat flux and flow field inside the reactor, and Chemical Reaction Engineering Module to examine the multiscale concentration distributions. Two models from the Application Libraries are also being referenced: "Shell and Tube Heat Exchanger" (ID: 12685), and "A Multiscale 3D Packed Bed Reactor" (ID: 17019).

Besides the heat and flow characteristics, macro- and micro-mass balances are also being coupled in this model by calculating the concentration profiles of reacting species from a multiscale perspective: a macroscale distribution for the gas flow in the 3D HI-Light reactor, as well as a microscale distribution inside each individual catalyst pellet. The extra dimension is being built in the feature Reactive Pellet Bed.

We anticipate that the HI-Light reactor will enable a great improvement in catalyst usage effectiveness, volumetric productivity, and reactor efficiency over the state-of-the-art, significantly increasing the commercial viability of the technology.